Temperature chaos in a replica symmetry broken spin glass model - A hierarchical model with temperature chaos -

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Abstract. – Temperature chaos is an extreme sensitivity of the equilibrium state to a change of temperature. It arises in several disordered systems that are described by the so called scaling theory of spin glasses, while it seems to be absent in mean field models. We consider a model spin glass on a tree and show that although it has mean field behavior with replica symmetry breaking, it manifestly has "strong" temperature chaos. We also show why chaos appears only very slowly with system size.

Introduction. – The fragility of the equilibrium state to an infinitesimal change of temperature is commonly referred to as "temperature chaos" [1]. Having such fragility away from a phase transition point probably requires the system to be frustrated, but whether temperature chaos actually arises in generic frustrated systems is still subject to controversy. In the context of spin glasses [2, 3], temperature chaos is shown to be present for models on Migdal-Kadanoff lattices [4, 5]. Furthermore, the standard scaling theories [6, 1, 7] suggest that this is a general property of glassy systems; in support of this, the Directed Polymer in a Random Medium [8] (DPRM), which is well described by the (spin glass) scaling theories, is known to have temperature chaos [9, 10]. On the other hand, the Random Energy Model [11] has no temperature chaos [12], and what happens in the Sherrington-Kirkpatrick (SK) mean-field model of spin glasses is still unclear. A replica calculation for the SK model suggests the presence of temperature chaos [12], but the numerics indicate no chaos or only very weak chaos [13, 14, 15]. Furthermore, a more recent calculation by Rizzo [16] shows that temperature chaos is absent in perturbation theory about the critical temperature $T_{\rm c}$ to the orders computed. To clarify this question of temperature chaos in mean-field spin glasses, in this paper we study a specific mean-field-like model. By determining the probability density of overlaps for two real replicas at two different temperatures, we show that this model has temperature chaos even though it has a mean field behavior with replica symmetry breaking. Our quantitative study also gives a coherent picture of chaos and suggests why chaos is so weak in general.

The model based on a tree. – In this paper, we focus on the model introduced in ref. [17]. It is very similar to the model of a polymer on a disordered Cayley tree studied by Derrida and Spohn [18] (see also [19, 20]); the differences are that values of both energy and entropy are assigned to each branch of the tree and each state thus has extensive entropy. It is also close to the Random-entropy Random-energy model [21]; however, the energies and entropies are assigned hierarchically and the entropy is not introduced in an ad-hoc way.

The model is constructed as follows. We consider a Cayley tree rooted at O. Each branch point B (including O) creates K branches which connect B to its descendants. A tree with L generations is obtained by repeating this procedure L times. We regard the leaves (the bottom points) of the tree as the states of the system. A tree with L generations has K^L states. A random energy ϵ and a random entropy σ are associated with every branch of the tree. The variables ϵ (respectively σ) are drawn independently from the same distribution $\rho_E(\epsilon)$ ($\rho_S(\sigma)$). The energy $E(B)$ (entropy $S(B)$) of a branch point B is given by summing up the ϵ's (σ's) of the branches which lie along the path connecting it to O. This means that the values of energy and entropy are correlated hierarchically. The distance d_{ij} of two states i and j is d ($d = 0, 1, \dots, L$) if their first common ancestor arises on the d-th layer counted from below. The overlap q_{ij} is related to d_{ij} by $q_{ij} = 1 - d_{ij}/L$, where L is the number of generations of the tree.

Note that our model is mapped onto Derrida and Spohn's model [18] if we set $\rho^*_E(\epsilon') \equiv \int \mathrm{d}\epsilon \mathrm{d}\sigma \delta(\epsilon' - \epsilon + T\sigma)\rho_E(\epsilon)\rho_S(\sigma)$. Therefore, we can use the results in ref. [18] whenever we consider observables which depend on just one temperature. (Of course the concern of this paper is almost exclusively observables associated with two temperatures.) A consequence of this mapping is that our model has a critical temperature T_c below which it exhibits one step replica symmetry breaking (RSB): when $T < T_c$, the distribution of overlaps consists of two delta function peaks, one at 0 and one at 1.

Derivation of the overlap distribution with two different temperatures. – To study temperature chaos in this model, consider a given realization of the quenched disorder (the random energies and entropies); for that disorder, introduce two real replicas at equilibrium, one at temperature T and the other at temperature T', both temperatures being below T_c. Of interest is the probability distribution of the overlap of these two replicas. We want to know how this distribution depends on L and on the temperatures. We thus calculate the disorder averaged "integrated probability" to find the two replicas at a distance less or equal to d. This probability is explicitly defined as

$$Y_{TT'}(L,d) \;\equiv\; \overline{\frac{1}{Z_T(L)Z_{T'}(L)} \sum\nolimits_{ij/d_{ij}\le d} \mathrm{e}^{-X_T(i)-X_{T'}(j)}}. \tag{1}$$

In this expression, $\overline{\cdots}$ represents the disorder average, $X_T(i) \equiv E(i)/T - S(i)$ is the free-energy divided by T of state i, and $Z_T(L)$ is the partition function at temperature T for L generations. Using an integral representation of $1/x$ for the two quantities $Z_T(L)$ and $Z'_T(L)$, we can rewrite eq. (1) as

$$Y_{TT'}(L,d) \;=\; \int_{-\infty}^{\infty} \mathrm{d}u\mathrm{d}v F_{TT'}(L,d;u,v), \tag{2}$$

$$F_{TT'}(L,d;u,v) \equiv \overline{\exp\left[-e^{-u}Z_T(L) - e^{-v}Z_{T'}(L) - u - v\right] \sum\nolimits_{ij/d_{ij}\le d} \mathrm{e}^{-X_T(i)-X_{T'}(j)}}. \tag{3}$$

We can use $\sum_{ij/d_{ij}\le d} \exp[-X_T(i) - X_{T'}(j)] = \sum_{B_d} \exp[-X_T(B_d) - X_{T'}(B_d)] z_T(B_d) z_{T'}(B_d)$, where B_d is a general branch point in the d-th layer (counted from below) and $z_T(B)$ is the

partition function at T of the sub-tree rooted at a branch point B, in order to obtain

$$
\begin{aligned}
F_{TT'}(L,d;u,v) \;\equiv\; & \overline{\exp\left[-e^{-u}Z_T(L)-e^{-v}Z_{T'}(L)-u-v\right]} \\
& \overline{\times\sum\nolimits_{B_d} \exp[-X_T(B_d)-X_{T'}(B_d)]z_T(B_d)z_{T'}(B_d)}. \qquad (4)
\end{aligned}
$$

From this equation, we find

$$
F_{TT'}(d,d;u,v) = H_{TT'}(d;1,1;u,v), \qquad (5)
$$

$$
H_{TT'}(d;m,n;u,v) \equiv \overline{[e^{-u}z_T(B_d)]^m[e^{-v}z_{T'}(B_d)]^n \exp\left[-e^{-u}z_T(B_d)-e^{-v}z_{T'}(B_d)\right]}. \qquad (6)
$$

We can calculate $H_{TT'}(d;m,n;u,v)$ (including $H_{TT'}(d;1,1;u,v)$ which appears in eq. (5)) by the following recursion formulae. For $m=n=0$, it is not so difficult to find

$$
\begin{aligned}
H_{TT'}(0;0,0;u,v) &= \exp[-e^{-u}-e^{-v}], & (7)\\
H_{TT'}(d+1;0,0;u,v) &= \tilde{H}_{TT'}(d;0,0;u,v)^K, & (8)
\end{aligned}
$$

where for a general two variable function $g(u,v)$, we have defined

$$
\tilde{g}(u,v) \equiv \int \mathrm{d}\epsilon \mathrm{d}\sigma \rho_E(\epsilon)\rho_S(\sigma) g(u+\epsilon/T-\sigma, v+\epsilon/T'-\sigma). \qquad (9)
$$

The recursion formula for general m and n is derived by applying the relation

$$
H_{TT'}(d;m,n;u,v) = \frac{\partial^m}{\partial u^m}\frac{\partial^n}{\partial v^n} H_{TT'}(d;0,0;u,v) \qquad (10)
$$

to eqs. (7) and (8). For example, the recursion formula for $H_{TT'}(d;1,0;u,v)$ is

$$
\begin{aligned}
H_{TT'}(d+1;1,0;u,v) &= \frac{\partial}{\partial u}\tilde{H}_{TT'}(d;0,0;u,v)^K \\
&= K\tilde{H}_{TT'}(d;1,0;u,v)\tilde{H}_{TT'}(d;0,0;u,v)^{K-1}. \qquad (11)
\end{aligned}
$$

Finally, a method similar to the one used in ref. [17] leads us to

$$
F_{TT'}(L+1,d;u,v) = K\tilde{F}_{TT'}(L,d;u,v)\tilde{H}_{TT'}(L;0,0;u,v)^{K-1} \qquad (L \geq d). \qquad (12)
$$

In summary, the disorder averaged distribution of distances $Y_{TT'}(L,d)$ can be computed by the following procedure: (i) Calculate $H_{TT'}(d;1,1;u,v)$ (=$F_{TT'}(d,d;u,v)$) by evaluating numerically the recursions which are derived by applying eq. (10) to eqs. (7) and (8). (ii) Calculate $F_{TT'}(L,d;u,v)$ by using the recursion eq. (12). (iii) Compute $Y_{TT'}(L,d)$ by estimating numerically the integral in eq. (2).

Temperature chaos. – To show that this model has temperature chaos, let us first measure $Y_{TT'}(L,d=0) = \overline{\sum_i P_T^{\mathrm{eq}}(i)P_{T'}^{\mathrm{eq}}(i)}$, where $P_T^{\mathrm{eq}}(i) = \exp[-X_T(i)]/Z_T$. This is a generalization of $\overline{\sum_i\{P_T^{\mathrm{eq}}(i)\}^2}$ which has been studied in many systems like the SK model [22] and the Random Energy Model [23]. The result is shown in Fig. 1 (A). We used $K=2$, $\rho_E(\epsilon) = 0.25\delta(\epsilon)+0.5\delta(\epsilon-1)+0.25\delta(\epsilon-2)$ and $\rho_S(\sigma) = 0.5\delta(\sigma)+0.5\delta(\sigma-4)$ for those data. The critical temperature T_{c} is around 1.63 by the mapping to the Derrida-Spohn model and using the corresponding formula in [18]. We see that $Y_{TT'}(L,d=0)$ decays exponentially for $T \neq T'$ while it converges to a non-zero value for $T=T'$. (More precisely, a fit of the data at large L gives $Y_{TT'}(L,d=0) \approx AL^{-1/2}\exp(-BL)$.) These results tell us that *the partition function*

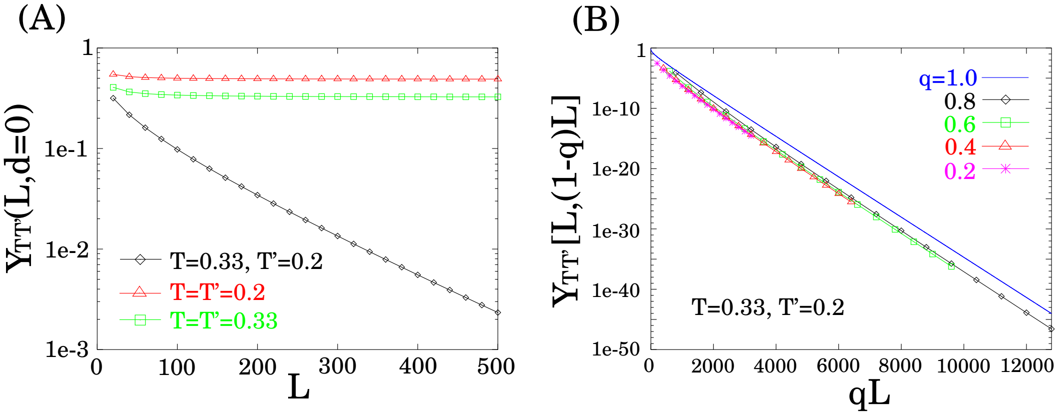

Fig. 1 – (A) $Y_{TT'}(L,d=0)$ vs. L for $(T,T')=(0.33,0.2)$, $(0.2,0.2)$ and $(0.33,0.33)$. The parameters for these data are $K=2$, $\rho_E(\epsilon)=0.25\delta(\epsilon)+0.5\delta(\epsilon-1)+0.25\delta(\epsilon-2)$ and $\rho_S(\sigma)=0.5\delta(\sigma)+0.5\delta(\sigma-4)$. The critical temperature T_c is around 1.63. (B) $Y_{TT'}(L,(1-q)L)$ for $(T,T')=(0.33,0.2)$ vs. qL. The data are taken for $q=0.2,0.4,0.6,0.8$ and 1.0 with the same parameters as before.

below T_c is dominated by a few states, but these dominant states change with temperature, i.e., there is temperature chaos. We have also checked that temperature chaos is absent in the model without entropy (no $\rho_S(\sigma)$); this is in agreement with ref. [12] which shows that the GREM does not have temperature chaos. Ref. [12] also has shown that there *is* chaos against magnetic field in the GREM. But this result is not so surprising if one notices that the energy of state i under field H is $E(i)-HM(i)$ ($M(i)$ is the magnetization of state i), and field plays the same role as temperature in our model.

The quantity $Y_{TT'}(L,d=0)$ decays "very fast", in fact exponentially with L, not as a stretched exponential or as a power of L. This suggests that the overlap probability distribution itself decays exponentially to zero for non-zero overlaps; to check this, we now study $Y_{TT'}(L,d)$. Interestingly, it turns out that $Y_{TT'}(L,d)$ satisfies the scaling law

$$Y_{TT'}(L,d) \approx \hat{Y}_{TT'}(L-d) \tag{13}$$

for large L and d. To show this, first rewrite eq. (1) as

$$Y_{TT'}(L,d) = \overline{\frac{\sum_{B_d} \exp\left[-X_T(B_d)-\delta f_T(B_d)-X_{T'}(B_d)-\delta f_{T'}(B_d)\right]}{\sum_{B_d,B'_d} \exp\left[-X_T(B_d)-\delta f_T(B_d)-X_{T'}(B'_d)-\delta f_{T'}(B'_d)\right]}}, \tag{14}$$

where $\delta f_T(B_d) \equiv -\log[z_T(B_d)] + \overline{\log[z_T(B_d)]}$. Derrida and Spohn [18] prove that $\delta f_T(B_d)$ has a limiting distribution that has a finite variance as $d\to\infty$. Furthermore, the statistics of $X_T(B_d)$ only depend on $L-d$. These facts lead us to the scaling law eq. (13).

The validity of eq. (13) is confirmed in Fig. 1 (B) where $Y_{TT'}(L,(1-q)L)$ for $q=0.2,0.4,0.6,0.8$ and 1.0 is plotted as a function of qL. Notice that $Y_{TT'}(L,(1-q)L)$ is the probability that the overlap of the two replicas is larger than q. The data, except those for $q=1$, satisfy the scaling very well (note that $Y_{TT'}(L,0)$ is calculated by eq. (14) with $\delta f_T=\delta f_{T'}=0$). Furthermore, we see that the slopes for $Y_{TT'}(L,0)$ and for the scaling function are the same. This means that the presence of δf_T in eq. (14) does not change the slope because the variance of δf_T is finite. Hereafter we regard the inverse of the exponent in this exponential decay as the chaos length $\ell(T,T')$ of the model.

This analysis shows that $\int_q^1 \mathrm{d}q' P_{TT'}(q')$ decays as $\exp[-qL/\ell(T,T')]$ if $q \neq 0$, meaning that $P_{TT'}(q)$ also decays (up to power corrections) exponentially. This property corresponds to "strong" chaos in any reasonable classification of chaos. To obtain some insight into the origin of the strong chaos, let us focus on $Y_{TT'}(L, d=0)$ which is the sum over all K^L states of $\exp[-\{F_T(i)-F_{\mathrm{eq}}(T)\}/T-\{F_{T'}(i)-F_{\mathrm{eq}}(T')\}/T']$. (In this expression, $F_T(i)$ is the free-energy of state i at temperature T and $F_{\mathrm{eq}}(T)$ is the equilibrium free-energy.) Now let us assume that among these K^L states it is enough to consider just those that dominate the partition function at some temperature T''. Since they are dominant states, the energy, the entropy and the free-energy of these states are the same as the equilibrium ones at T''. Therefore, at any temperature T_{m} the free-energy $F_{T_{\mathrm{m}}}(i)$ of these states are $E_{\mathrm{eq}}(T'') - T_{\mathrm{m}} S_{\mathrm{eq}}(T'')$ $(= F_{\mathrm{eq}}(T'') - S_{\mathrm{eq}}(T'')(T_{\mathrm{m}} - T''))$. On the other hand, the Taylor expansion of $F_{\mathrm{eq}}(T_{\mathrm{m}})$ around T'' leads us to $F_{\mathrm{eq}}(T_{\mathrm{m}}) = F_{\mathrm{eq}}(T'') - S_{\mathrm{eq}}(T'')(T_{\mathrm{m}} - T'') - \frac{1}{2T''}C(T'')(T_{\mathrm{m}} - T'')^2 + \mathcal{O}((T_{\mathrm{m}} - T'')^3)$, where C is the heat capacity. By using this for $T_{\mathrm{m}} = T$ or T', we find that the contribution to $Y_{TT'}(L, d=0)$ for such a state is $\exp[-\{(T-T'')^2/T + (T'-T'')^2/T'\}C(T'')/(2T'')]$. For $\Delta T \equiv T - T' \ll 1$, this is maximized at $T'' = \frac{T+T'}{2}$ and we obtain

$$Y_{TT'}(L, d=0) \approx \exp[-\Delta T^2 C(T)/(4T^2)]. \tag{15}$$

In our model, C grows linearly with L, leading to an exponential decay of $Y_{TT'}(L, d=0)$ with L. On the contrary, the specific heat in the low temperature phase is zero in the REM [11] and in our model without entropy [18] and thus there is no chaos in these systems.

Interestingly, this computation is only qualitatively correct and eq. 15 does *not* give the exact overlap length. The reason is that we have relied on typical contributions to $Y_{TT'}$ while in fact it is dominated by rare events: a tiny fraction of the samples where the same state is dominant at T and T' determine the disorder averaged probability $Y_{TT'}$. To calculate the true $\ell(T,T')$, we have to take into account such rare events; to do so, we first study how fluctuations grow with L at a given temperature.

Scaling of the entropy fluctuations. – In Fig. 2, we show the fluctuations of entropy, energy and free-energy which are defined as

$$\sigma_T^2(\mathcal{O}) = \overline{\langle \mathcal{O}^2 \rangle_T} - \left\{ \overline{\langle \mathcal{O} \rangle_T} \right\}^2, \tag{16}$$

where $\mathcal{O}$ is quantity associated with *each* state, i.e., energy, free-energy and entropy, and

$$\langle \mathcal{O} \rangle_T \equiv \frac{\sum_i \mathcal{O}(i) \exp[-X_T(i)]}{Z_T(L)}. \tag{17}$$

These quantities were calculated by recursion formulae similar to the ones for $Y_{TT'}$. We clearly see that $\sigma_T^2(S)$ and $\sigma_T^2(E)$ grow linearly with L, while $\sigma_T^2(F)$ converges to a finite value. These results show that there are a few states which have almost the same lowest free-energy, but whose entropies are very different from one-another. Therefore, the relative order of these dominant states can change by a small change of the temperature, i.e., the free-energy levels can cross, and these kinds of crossings generate temperature chaos in this model. Note that this mechanism of temperature chaos was first proposed in the scaling theories [6, 1, 7] and its validity is also confirmed in other systems [10, 21]. It is also worth noticing that $\Delta S(i,T) \equiv S(i) - \overline{\langle S \rangle_T}$ and $\Delta E(i,T)$ are strongly correlated for the dominant states so that $\Delta S(i,T) \approx \Delta E(i,T)/T$ because of the relation $\Delta F(i,T) = \Delta E(i,T) - T\Delta S(i,T)$. This is the reason why $\sigma_T^2(S)$ and $\sigma_T^2(E/T)$ are almost the same in Fig. 2.

The same results hold for state-to-state fluctuations defined as $\hat{\sigma}_T^2(\mathcal{O}) \equiv \overline{\langle \mathcal{O}^2 \rangle_T} - \overline{\langle \mathcal{O} \rangle_T^2}$. First, $\hat{\sigma}_T^2(F)$ stays $O(1)$ since $\hat{\sigma}_T^2(F) \leq \sigma_T^2(F)$. Second, $\hat{\sigma}_T^2(E)$ grows linearly with L because $\hat{\sigma}_T^2(E)$ is proportional to the heat capacity. From these two results, $\hat{\sigma}_T^2(S) \approx \hat{\sigma}_T^2(E/T) \propto L$.

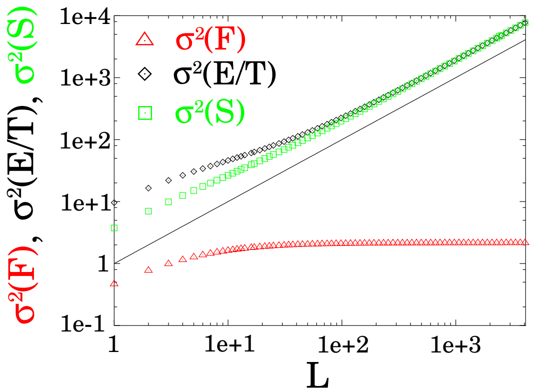

Fig. 2

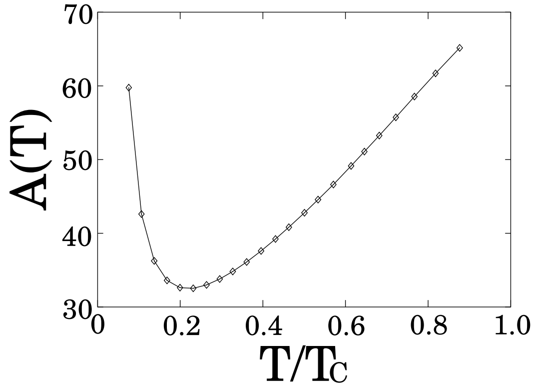

Fig. 3

Fig. 2 – Fluctuations of energy, entropy and free-energy at $T = 0.2$ vs. generation L. The parameters are the same as in Fig. 1. A function linear in L is drawn to guide the eye.

Fig. 3 – A(T) vs. $T/T_{\rm c}$ using the same parameters as Fig. 1. $A(T)$ is defined in eq. (22).

Consequences for the overlap length. – Let us estimate $Y_{TT'}(L,0)$ to calculate $\ell(T,T')^{-1}$ (recall that $Y_{TT'}(L,0) \sim \exp[-L/\ell(T,T')]$). We denote the state with the lowest free-energy at T by D_T. If $F_{T'}(D_T) = E(D_T) - T'S(D_T)$ happens to be smaller than $\overline{\langle F\rangle_{T'}}$, the dominant state at T' is still D_T ($D_{T'} = D_T$) so that $Y_{TT'}(L,0)$ for that sample is of order 1. Therefore,

$$\begin{aligned} Y_{TT'}(L,0) &\approx \mathrm{Prob}(F_{T'}(D_T) \le \langle F\rangle_{T'}) \\ &= \mathrm{Prob}\Big((T-T')\Delta E(D_T,T) \le T[\overline{\langle F\rangle_{T'}} - \overline{\langle F\rangle_T} - (T-T')\overline{\langle S\rangle_T}]\Big), \end{aligned} \tag{18}$$

where we have used $\Delta S(i,T) \approx \Delta E(i,T)/T$ to go from the first line to the second. Now assume that the distribution of $\Delta E(D_T,T)$ is Gaussian; this seems to be plausible since $\sigma_T(E)$ is linear in L, as if there was an underlying central limit theorem process. Then we obtain

$$Y_{TT'}(L,0) \sim \{L/\ell(T,T')\}^{-\frac{1}{2}} \exp[-L/\ell(T,T')], \tag{19}$$

$$\ell(T,T') = \frac{2\sigma_T^2(E)L(T-T')^2}{T^2\left[\overline{\langle F\rangle_{T'}} - \overline{\langle F\rangle_T} - (T-T')\overline{\langle S\rangle_T}\right]^2}. \tag{20}$$

The accuracy of eq. (20) was checked by comparing $\ell(T,T')$ estimated from $Y_{TT'}(L,0)$ and from eq. (20). The result was very satisfactory, i.e., the former is 131.3 and the latter 131.8 when the parameters are those used in Fig. 1. We also found similarly good accuracy for the other sets of (T,T') we tested. From eq. (20), we find

$$\ell(T,T+\Delta T) \approx A(T)\left(\frac{\Delta T}{T}\right)^{-2} \qquad (\Delta T \ll 1), \tag{21}$$

$$A(T) = 8\sigma_T^2(E)C(T)^{-2}T^{-2}L, \tag{22}$$

where again $C(T)$ is the heat capacity ([1]). It should be noted that the chaos exponent ζ defined via $\ell(T,T+\Delta T) \approx (\Delta T)^{-1/\zeta}$ is correctly given by the droplet theory [7, 10] which

([1])Rigorously speaking, eq. (22) is valid when $\overline{\langle F\rangle_T}/L = -k_{\rm B}T\overline{\log Z(T)}/L$. This relation is justifiable in the low temperature phase where only a few states dominate thermodynamics of the system, and we have checked this numerically.

predicts $\zeta = \frac{d_s - 2\theta}{2}$ if $\hat{\sigma}_T^2(S) \propto L^{d_s}$ and $\hat{\sigma}_T^2(F) \propto L^{2\theta}$. (Indeed, Fig. 2 shows $d_s = 1$ and $\theta = 0$ in this model). Figure 3 shows $A(T)$ of the model. We find that $A(T)$ has a minimum around $T \approx 0.2$ for which the value is about 33. This tells us that temperature chaos emerges only at large scales, e.g., when temperature is changed by 10% ($\frac{\Delta T}{T} = 0.1$), the chaos length is at least 3300. But note that eqs. (21) and (22) give us chaos *volume* if we consider the case $d \neq 1$ since L is volume in this model. (Remember that energy and entropy are proportional to L.) Therefore, the minimum chaos *length* for $\frac{\Delta T}{T} = 0.1$ is not so large for $d = 3$, i.e., $3300^{1/3} \approx 15$.

Conclusions. – We have studied a GREM-like system with extensive entropy; it has strong temperature chaos, $P_{TT'}(q)$ decaying as $\exp[-qL/\ell(T,T')]$ if $T \neq T'$. Entropy fluctuations from valley to valley are the central ingredients for temperature chaos, as predicted by the scaling (droplet) theory [6, 1, 7]. Note that the overlap length $l(T,T')$ is proportional to $C(T)^{-1}(T-T')^{-2}$ (see eqs. (15) and (22)) and that $C(T)$ is typically small. If $C(T)$ controls the decay of overlap probability in more general disordered systems also, then it is no surprise that temperature chaos is difficult to detect in simulations. Finally rejuvenation and memory effects observed in off-equilibrium dynamics [24, 25] are naturally interpreted by this model because it has both temperature chaos and a hierarchical structure. Consider for example the case where temperature is changed as $T \to T - \Delta T \to T$. A strong *rejuvenated* relaxation will be observed at $T - \Delta T$ due to temperature chaos, while memory will emerge when the temperature is returned to T because of the hierarchical structure.

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